Mandelic acid
90-64-2 | DTXSID6023234

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.82 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.26e-01

Confidence level: 5.94e-01

Nearest Neighbors from the Training Set

Image not found 1-Hydroxycyclohexanecarboxylic acid **Measured:** 4.65e-01 **Predicted:** 3.19e-01	Image not found 2-Ethyl-2-nitro-1,3-propanediol **Measured:** 6.71 **Predicted:** 4.94	Image not found Bronopol **Measured:** 1.25 **Predicted:** 2.20
Image not found Mandelic acid **Measured:** 1.14 **Predicted:** 1.82	Image not found Mandelic acid **Measured:** 1.14 **Predicted:** 1.82	Image not found Mandelic acid **Measured:** 1.14 **Predicted:** 1.82
Image not found Mandelic acid **Measured:** 1.14 **Predicted:** 1.82	Image not found 2-Methyl-2-nitro-1,3-propanediol **Measured:** 5.92 **Predicted:** 5.43	